Surface Diffraction Study of Protein Crystals

S. Boutet, I. Robinson (U. of Illinois), Z. Hu, W. Thomas and A. Chernov (Marshall Research Center)

Abstract No. Bout6701
Beamline(s): **X16C**

We attempted the first measurement of a Crystal Truncation Rod (CTR) from a protein crystal. This measurement was performed as a first step toward a deeper study of surfaces and growth of crystals of proteins using X-rays. The protein studied in this case was Holoferritin, the iron-filled version of the iron storage protein Ferritin, which is a large spherical shell (diameter 130Å). This protein crystallizes in the FCC structure with lattice parameter a=184Å. The crystals have a convenient octahedral morphology making the {111} surfaces easy to locate.

We studied a series rocking curves of the crystal cutting across the CTR above and below the 111 bulk reflection. One such series is shown on Figure 1. As the orientation of the crystal is varied (angle ω), the truncation rod appears as a peak in the center of each scan. The series shows a rapid falloff of the intensity of this center peak as the scans move away from the bulk reflection. This falloff is characteristic of CTR, although much more rapid in this case than for previously studied inorganic crystal surfaces, possibly showing a high level of disorder and roughness of the protein crystal.

Most of the rocking curves also display a second and third peak, along with the peak from the CTR. These two extra peaks are found to be symmetric on each side of the CTR peak. Close examination revealed that the first of the two extra peaks always appears at the same ω value, while the second peak appears at the same value of the quantity 2θ-ω. We believe, from simple geometric arguments shown in Figure 2 that the first peak arises from forward scattering of the outgoing diffracted beam, when the incident beam satisfies the Bragg condition. The large intensity of the diffracted beam allows for a few X-rays to be scattered into the detector. As for the second peak, it arises from multiple scattering of the incident beam into the Bragg condition. The few X-rays scattered in such a way then meet the Bragg condition and diffract from the crystal into the detector. Then this peak arises when the outgoing beam satisfies the Bragg condition.

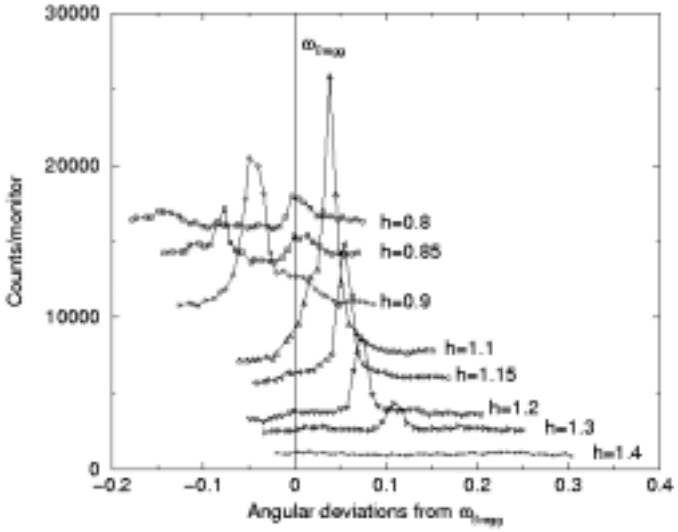

Figure 1. Rocking curves crossing different points on the (h,h,h) CTR. The value of ω=0 corresponds to the Bragg condition on the incident beam.

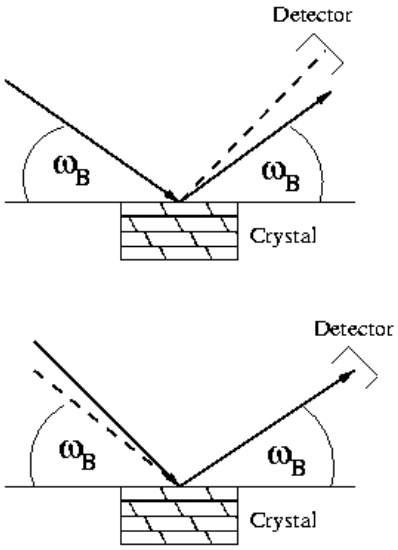

Figure 2. Model showing how forward scattering creates the two extra peaks observed. Top : The Bragg condition on the incident beam is met, which means a large intensity is diffracted (solid line). Some X-rays of the diffracted beam scatter into the detector (dashed line). Bottom : The Bragg condition is met on the diffracted beam and some of the X-rays in the incident beam scatter into the Bragg condition (dashed line) and are then diffracted by the crystal.